Comparison of Low Field Electron Transport Characteristics in InP,GaP,Ga$_{0.5}$In$_{0.5}$P and In As$_{0.8}$P$_{0.2}$ by Solving Boltzmann Equation Using Iteration Model

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Abstract

Temperature and doping dependencies of electron mobility in InP, GaP and Ga0.52In0.48P structures have been calculated using an iterative technique. The following scattering mechanisms, i.e, impurity, polar optical phonon, acoustic phonon and piezoelectric are included in the calculation. Ionized impurity scattering has been treated beyond the Born approximation using the phase-shift analysis. It is found that the electron mobility decreases monotonically as the temperature increases from 100K to 500K for each material which is depended to their band structures characteristics. The low temperature value of electron mobility increases significantly with increasing doping concentration. The iterative results are in fair agreement with other recent calculations obtained using the relaxation-time approximation and experimental methods.

KEYWORDS: Iterative technique; Ionized impurity scattering; Born approximation; electron mobility.

INTRODUCTION

The ternary semiconductor, Ga$_{0.5}$In$_{0.5}$P offers a large direct band gap of the III-V compound semiconductor material which is lattice matched to a commonly available substrate like GaP or InP. Owing to its relatively large band gap, this material has been cited for its potential use in visible light emitters such as light emitting diodes and lasers [7-8]. Ga0.52In0.48P has further potential usage as a visible light detector as well as in high temperature and/or high power electronics. The problems of electron transport properties in semiconductors have been extensively investigated both theoretically and experimentally for many years. Many numerical methods available in the literature (Monte Carlo method, Iterative method, variation method, Relaxation time approximation, or Mattiessen's rule) have lead to approximate solutions to the Boltzmann transport equation [1,2]. However, carrier transport modeling of Ga0.50In0.50P materials has only recently begun to receive sustained attention, now that the growth of compounds and alloys is able to produce valuable material for the electronics industry. In this communication we present iterative calculations of electron drift mobility in low electric field application. Because of high mobility InP has become an attractive material for electronic devices of superior performance among the III phosphates semiconductors (Besikci et al., 2000).Therefore study of the electron transport in group III phosphates is necessary. GaP possesses an indirect band gap of 0.6 eV at room temperature whereas InP have a direct band gap about 1.8 eV, respectively.

The low-field electron mobility is one of the most important parameters that determine the performance of a field-effect transistor. The purpose of the present paper is to calculate electron mobility for various temperatures and ionized-impurity concentrations. The formulation itself applies only to the central valley conduction band. We have also considered band nonparabolicity and the screening effects of free carriers on the scattering probabilities. All the relevant scattering mechanisms, including polar optic phonons, deformation potential, piezoelectric, acoustic phonons, and ionized impurity scattering. The Boltzmann equation is solved iteratively for our purpose, jointly incorporating the effects of all the scattering mechanisms [3,4].This paper is organized as follows. Details of the iteration model , the electron scattering mechanism which have been used and the electron mobility calculations are presented in section II and the results of iterative calculations carried out on Inp,Gap,Ga$_{0.5}$ In$_{0.5}$P and InAs$_{0.8}$P$_{0.2}$ structures are interpreted in section III.

II. Model detail

To calculate mobility, we have to solve the Boltzmann equation to get the modified probability distribution function under the action of a steady electric field. Here we have adopted the iterative technique for solving the Boltzmann transport equation. Under the action of a steady field, the Boltzmann equation for the distribution function can be written as

$$\frac{\partial f}{\partial t} + v.\nabla_r f + \frac{eF}{\hbar}.\nabla_k f = (\frac{\partial f}{\partial t})_{coll} \qquad (1)$$

Where $(\partial f / \partial t)_{coll}$ represents the change of distribution function due to the electron scattering. In the steady-state and under application of a uniform electric field the Boltzmann equation can be written as

$$\frac{eF}{\hbar}.\nabla_k f = (\frac{\partial f}{\partial t})_{coll}$$

Consider electrons in an isotropic, non-parabolic conduction band whose equilibrium Fermi distribution function is $f_0(k)$ in the absence of electric field. Note the equilibrium distribution $f_0(k)$ is isotropic in k space but is perturbed when an electric field is applied. If the electric field is small, we can treat the change from the equilibrium distribution function as a perturbation which is first order in the electric field. The distribution in the presence of a sufficiently small field can be written quite generally as

$$f(k) = f_0(k) + f_1(k)\cos\theta \qquad (3)$$

Where θ is the angle between k and F and $f_1(k)$ is an isotropic function of k, which is proportional to the magnitude of the electric field. f(k) satisfies the Boltzmann equation 2 and it follows that:

$$\frac{eF}{\hbar}\frac{\partial f_0}{\partial t} = \sum_i \left\{ \int \cos\varphi f_1' \left[S_i'(1-f_0) + S_i f_0 \right] d^3k - f_1 \int \left[S_i(1-f_0') + S_i' f_0' \right] d^3k' \right\} \quad (4)$$

In general there will be both elastic and inelastic scattering processes. For example impurity scattering is elastic and acoustic and piezoelectric scattering are elastic to a good approximation at room temperature. However, polar and non-polar optical phonon scattering are inelastic. Labeling the elastic and inelastic scattering rates with subscripts el and inel respectively and recognizing that, for any process i, $s_{eli}(k', k) = s_{eli}(k, k')$ equation 4 can be written as

$$f_1(k) = \frac{\frac{-eF}{\hbar}\frac{\partial f_0}{\partial k} + \sum \int f_1'\cos\phi \, [S_{inel}'(1-f_0) + S_{inel}f_0]d^3k'}{\sum \int (1-\cos\phi)S_{el}d^3k' + \sum \int [S_{inel}(1-f_0) + S_{inel}'f_0']d^3k'} \quad (5)$$

Note the first term in the denominator is simply the momentum relaxation rate for elastic scattering. Equation 5 may be solved iteratively by the relation

$$f_{1n}(k) = \frac{\frac{-eF}{\hbar}\frac{\partial f_0}{\partial k} + \sum \int f_1'\cos\phi \, [n-1][S_{inel}'(1-f_0) + S_{inel}f_0]d^3k'}{\sum \int (1-\cos\phi)S_{el}d^3k' + \sum \int [S_{inel}(1-f_0) + S_{inel}'f_0']d^3k'} \quad (6)$$

Where $f_{1n}(k)$ is the perturbation to the distribution function after the n-th iteration. It is interesting to note that if the initial distribution is chosen to be the equilibrium distribution, for which $f_1(k)$ is equal to zero, we get the relaxation time approximation result after the first iteration. We have found that convergence can normally be achieved after only a few iterations for small electric fields. Once $f_1(k)$ has been evaluated to the required accuracy, it is possible to calculate quantities such as the drift mobility μ, which is given in terms of spherical coordinates by

$$\mu = \frac{\hbar}{3m^*F} \frac{\int_0^\infty (k^3/1+2\alpha F)f_1 d^3k}{\int_0^\infty k^2 f_0 d^3k} \qquad (7)$$

Here, we have calculated low field drift mobility in III-V structures using the iterative technique. In the following sections electron-phonon and electron-impurity scattering mechanisms will be discussed.

Deformation potential scattering The acoustic modes modulate the inter atomic spacing. Consequently, the position of the conduction and valence band edges and the energy band gap will vary with position because of the sensitivity of the band structure to the lattice spacing. The energy change of a band edge due to this mechanism is defined by a deformation potential and the resultant scattering of carriers is called deformation potential scattering. The energy range involved in the case of scattering by acoustic phonons is from zero to 2vk$\hbar$, where v is the velocity of sound, since momentum conservation restricts the change of phonon wave vector to between zero and 2k, where k is the electron wave vector. Typically, the average value of k is of the order of 10^7 cm^{-1} and the velocity of sound in the medium is of the order of 10^5 cms^{-1}. Hence, 2vk$\hbar$ ~ 1 meV, which is small compared to the thermal energy at room temperature. Therefore, the deformation potential scattering by acoustic modes can be considered as an elastic process except at very low temperature. The deformation potential scattering rate with either phonon emission or absorption for an electron of energy E in a non-parabolic band is given by Fermi's golden rule as [3,5]

$$R_{de} = \frac{\sqrt{2}D^2_{ac}(m_t^{*2}m_l^*)^{1/2}K_BT}{\pi\rho v^2\hbar^4}\frac{\sqrt{E(1+\alpha E)}}{E(1+2\alpha E)}$$
$$\left[(1+\alpha E)^2 + 1/3(\alpha E)^2\right]$$
$$(8)$$

Where D_{ac} is the acoustic deformation potential, ρ is the material density and α is the non-parabolicity coefficient. The formula clearly shows that the acoustic scattering increases with temperature

Piezoelectric scattering
The second type of electron scattering by acoustic modes occurs when the displacements of the atoms create an electric field through the piezoelectric

effect. The piezoelectric scattering rate for an electron of energy E in an isotropic, parabolic band has been discussed by Ridley [4] .

The expression for the scattering rate of an electron in a non-parabolic band structure retaining only the important terms can be written as [3,5]:

$$R_{PZ}(k) = \frac{e^2 K_B T K_{av}^2 \sqrt{m^*}}{2\sqrt{2}\pi \hbar^2 \varepsilon_s} \gamma^{-1/2} (1 + 2\alpha\varepsilon)$$

$$\left[(1 + \alpha\varepsilon)^2 + \frac{1}{3}(\alpha\varepsilon)^2 \right]$$

$$(9)$$

Where ε_s is the relative dielectric constant of the material and K_{av} is the dimensionless so called average electromechanical coupling constant .

Polar optical phonon scattering

The dipolar electric field arising from the opposite displacement of the negatively and positively charged atoms provides a coupling between the electrons and the lattice which results in electron scattering. This type of scattering is called polar optical phonon scattering and at room temperature is generally the most important scattering mechanism for electrons in III-V .The scattering rate due to this process for an electron of energy E in an isotropic, non-parabolic band is [3,5]

$$R_{PO}(\vec{k}) = \frac{e^2 \sqrt{2m^*} \omega_{PO}}{8\pi\varepsilon_\circ \hbar} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_\circ} \right) \frac{(1 + 2\alpha E)}{\sqrt{\gamma(E)}}$$

$$F_{PO}(E, E')\{N_{op}, N_{op} + 1\} \qquad (10)$$

Where $E = E' \pm \_w_{po}$ is the final state energy phonon absorption (upper case) and emission (lower case) and Nop is the phonon occupation number and the upper and lower cases refer to absorption and emission, respectively. For small electric fields, the phonon population will be very close to equilibrium so that the average number of phonons is given by the Bose- Einstein distribution.

Impurity scattering

This scattering process arises as a result of the presence of impurities in a semiconductor. The substitution of an impurity atom on a lattice site will perturb the periodic crystal potential and result in scattering of an electron. Since the mass of the impurity greatly exceeds that of an electron and the impurity is bonded to neighboring atoms, this scattering is very close to being elastic. Ionized impurity scattering is dominant at low temperatures because, as the thermal velocity of the electrons decreases, the effect of long-range Coulombic interactions on their motion is increased. The electron scattering by ionized impurity centers has been discussed by Brooks Herring [6] who included the modification of the Coulomb potential due to free carrier screening. The screened Coulomb potential is written as

$$V(r) = \frac{e^2}{4\pi \varepsilon_0 \varepsilon_s} \frac{\exp(-q_0 r)}{r} \qquad (11)$$

Where ε_s is the relative dielectric constant of the material and q_0 is the inverse screening length, which under no degenerate conditions is given by

$$q_0^2 = \frac{ne^2}{\varepsilon_0 \varepsilon_s K_B T} \qquad (12)$$

Where n is the electron density. The scattering rate for an isotropic, nonparabolic band structure is given by [3,5]

$$R_{im} = \frac{N_i e^4 (1 + 2\alpha E)}{32\sqrt{2m^*}\pi \varepsilon_s^2 (\gamma(E))^{3/2}} \left[Ln(1+b) - \frac{b}{1+b} \right] \qquad (13)$$

$$b = \frac{8m^* \gamma(E)}{\hbar^2 q_0^2} \qquad (14)$$

Where N_i is the impurity concentration.

III. RESULTS

We have performed a series of low-field electron mobility calculations for Inp,Gap,Ga $_{0.5}$In $_{0.5}$P and InAs$_{0.8}$P$_{0.2}$ materials. Low-field motilities have been derived using iteration method. The electron mobility is a function of temperature and electron concentration.

	GaP	InP	$Ga_{0.5}In_{0.5}P$	$InAs_{0.8}P_{0.2}$
m*	0.3m	0.073	0.105	0.036
Nonparabolicity(ev)	0.2	0.7	0.45	2.26
Density ρ(gr cm--3)	4.138	4.810	4.470	5.496
Longitudinal sound velocity vs(10^5cms--1)	5.850	5.3	4.33	4.484
Low-frequency dielectric constant ε0	11.1	12.4	11.75	14.16
High-frequency dielectric constant ε∞	9.11	9.55	9.34	11.71
Polar optical phonon energy (eV)	0.051	0.06	0.045	0.024
Acoustic deformation potential D(eV)	3.1	8.3	7.2	5.58

Figures 1 shows the comparison the electron mobility depends on the Temperature at the different electron concentration in bulk Gap,GaAs,InP and InAs materials. Figure 1 shows that electrons mobility at the definite temperature 300 k for the Inp semiconductors is gained about 11606 $cm^2v^{-1}s^{-1}$ and for Gap,$Ga_{0.5}In_{0.5}P$ and $InAs_{0.8}P_{0.2}$ about 5020,8960 and 26131 $cm^2v^{-1}s^{-1}$. Also electrons mobility decrease quickly by temperature increasing from 200 to 500 K for all the different electron concentrations because temperature increasing causes increase of phonons energy too. So it causes a strong interaction between electrons and these phonons that its result is increase of electrons scattering rate and finally decrease of electrons mobility. Our calculation results show that the electron mobility $InAs_{0.8}P_{0.2}$ is more than 3other materials this increasing is because of small effective mass.

and $InAs_{0.8}P_{0.2}$ at the electron concentration 10^{16} (cm-3).

Figure 2 shows the calculated variation of the electron drift mobility as a function of free electron concentration for all crystal structures at room temperature. The mobility does not vary monotonically between free electron concentrations of 10^{16} cm-3 and 10^{18} cm-3.Our calculation results show that the electron mobility $InAs_{0.8}P_{0.2}$ is
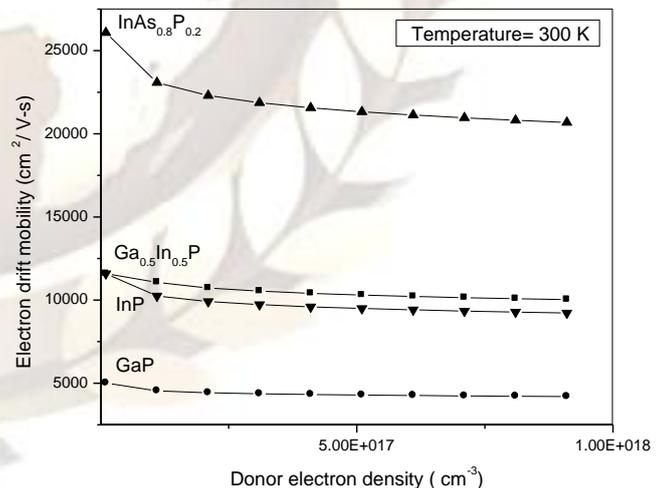
Fig 2. Changes the electron mobility Function in terms of room temperature in bulk Inp,Gap,$Ga_{0.5}In_{0.5}P$ and $InAs_{0.8}P_{0.2}$ at the different electron concentration.

Fig 1. Changes the electron mobility Function in terms of temperature in bulk Inp,Gap,$Ga_{0.5}In_{0.5}P$
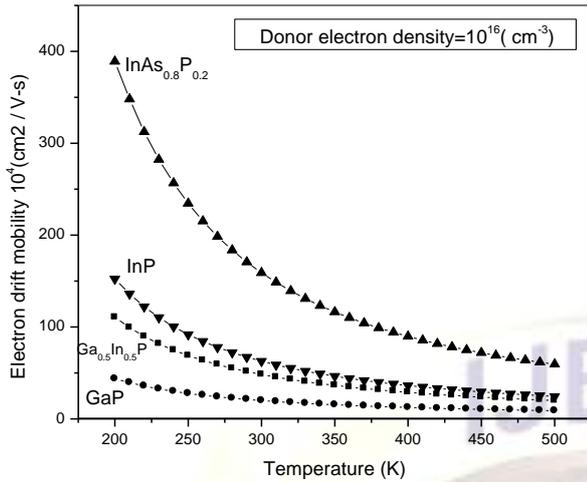
Fig.4. Electron drift mobility versus temperature in Inp,Gap,Ga $_{0.5}$In $_{0.5}$P and InAs$_{0.8}$P$_{0.2}$ with including inelastic scattering
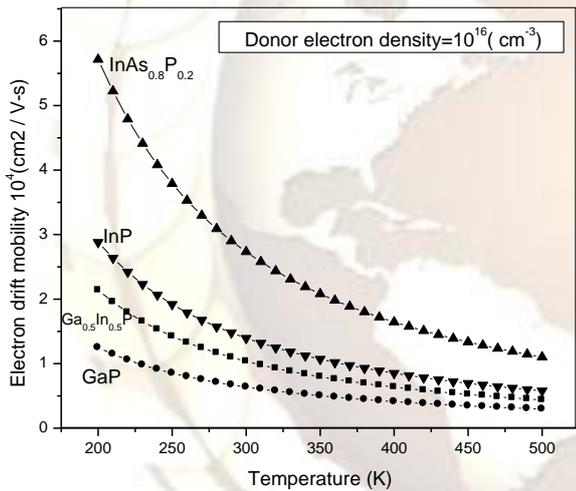
Fig.5. Electron drift mobility versus temperature in Inp,Gap,Ga $_{0.5}$In $_{0.5}$P and InAs$_{0.8}$P$_{0.2}$ with including elastic scattering.

CONCLUSION

In conclusion, we have quantitatively obtained temperature-dependent and electron concentration dependent electron mobility in Inp,Gap,Ga $_{0.5}$In $_{0.5}$P and InAs$_{0.8}$P$_{0.2}$ materials using an iterative technique. The theoretical values show good agreement with recently obtained experimental data. InAs$_{0.8}$P$_{0.2}$ semiconductor having high mobility of Inp,Gap and Ga $_{0.5}$In $_{0.5}$P because the effective mass is small compared with all of them . The ionized impurity scattering in all the Gap,Ga $_{0.5}$In $_{0.5}$P and InAs$_{0.8}$P$_{0.2}$ at all temperatures is an important factor in reducing the mobility.

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